Advanced Regression 4b: Machine learning, ensemble methods

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Ensemble methods:

- Bagging
- Random forests
- Boosting
- Variable importance
- Ensemble methods in `R`

Bootstrap aggregation (bagging)

- Let the original dataset contain n samples
- Take $n' < n$ repeated samples (with replacement) of the original dataset to create B new datasets ($b \in 1, ..., B$ bootstrapped training datasets).
- Grow a tree on each bootstrapped training datasets.
- Each of the trees has little bias, but high variance.

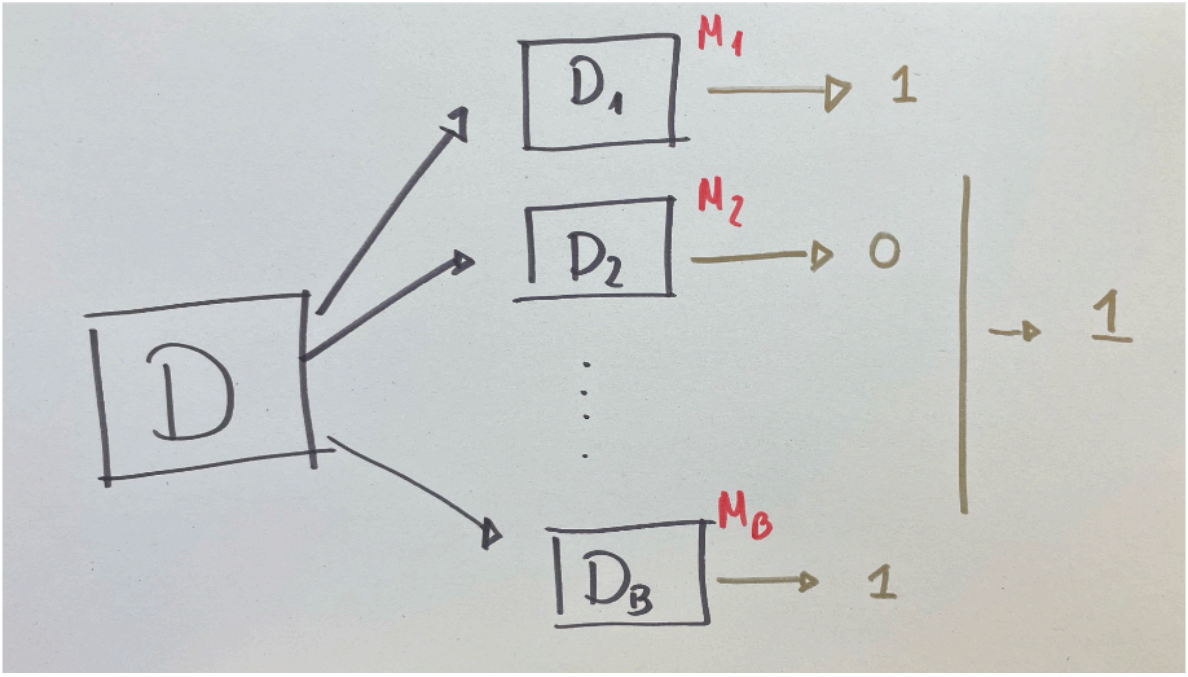
Average over trees

- Regression tree: Compute the mean over the B predictions f_b of each individual regression tree

$$f_{bag}(x) = \frac{1}{B}\sum_{b=1}^{B} f_b(x)$$

- Classification tree: Majority vote (mode), the final prediction is the one that occurred most frequently among the B trees

Bagging



Example (taken from Prof Filippi lecture)

- Aim: predict median house prices (Boston) based only on crime rate
- Consider a tree with a single split at the root

```
Warning: Using `size` aesthetic for lines was deprecated in ggplot2 3.4.0.
i Please use `linewidth` instead.
```

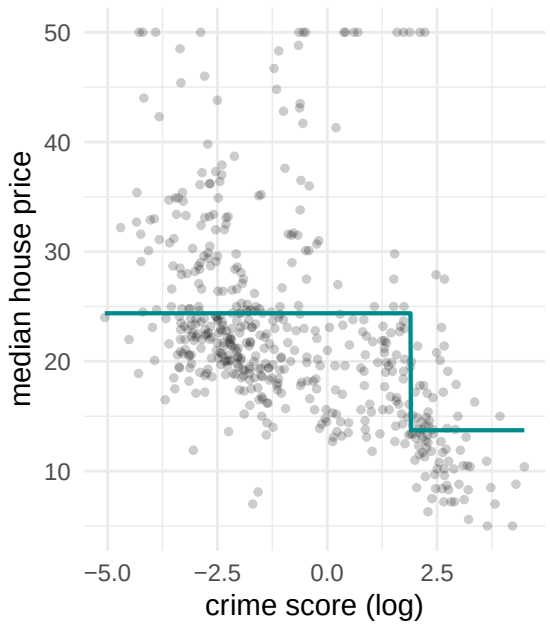
Example (taken from Prof Filippi lecture)

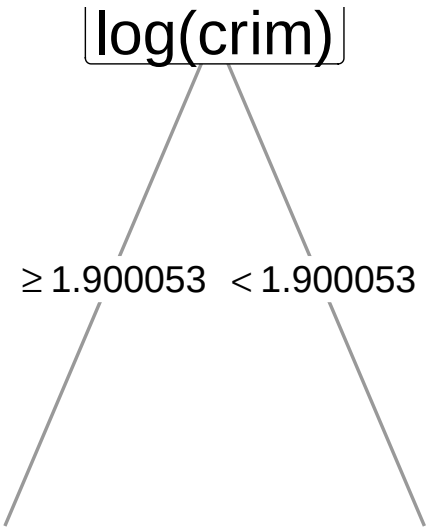
20 bootstrap samples

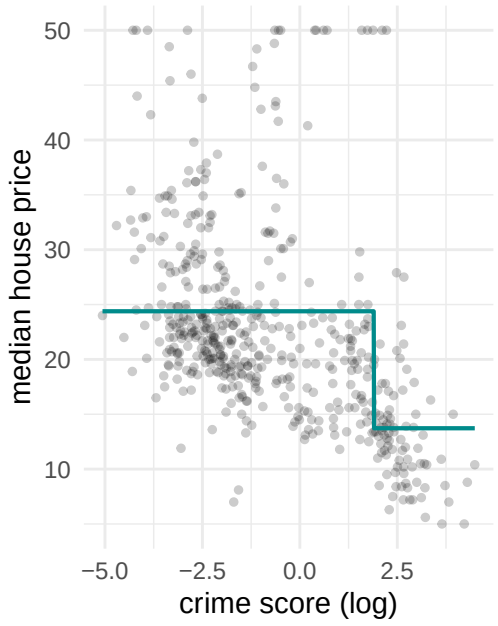
Example (taken from Prof Filippi lecture)

Summarise the samples

```
Joining with `by = join_by(row)`
```


median house price
50
40
30
20
10
−5.0
−2.5
0.0
2.5
crime score (log)


log(crim)
≥ 1.900053
< 1.900053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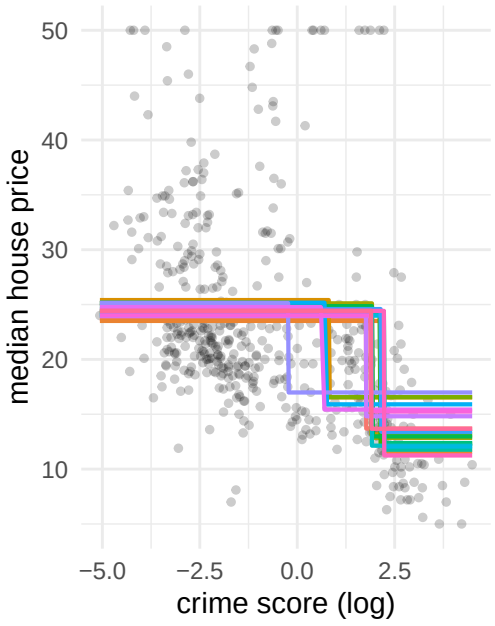
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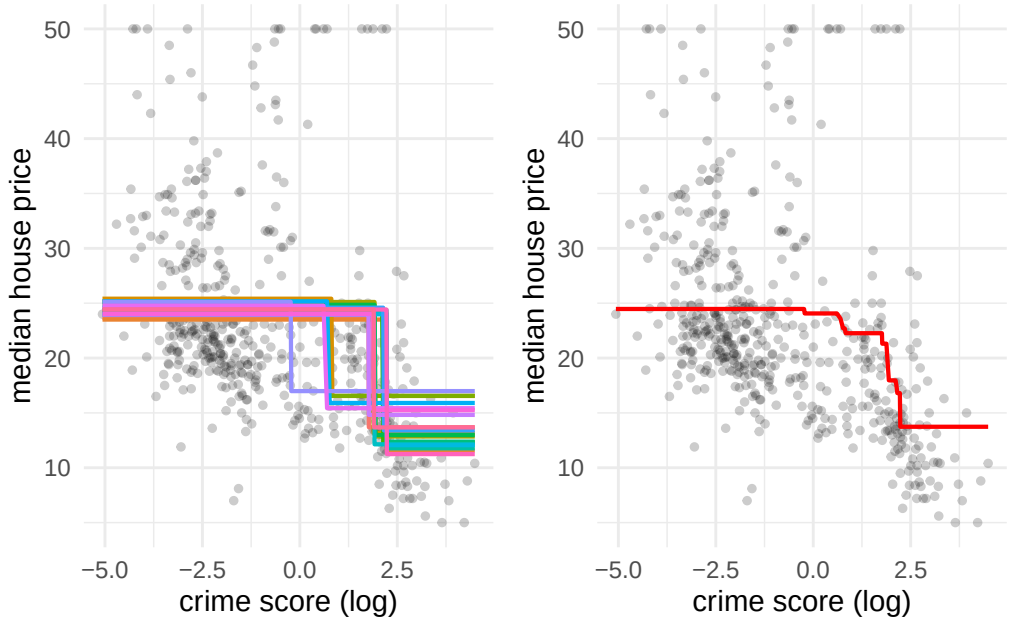


Out-of-bag error

- Bagging has an intrinsic way of evaluating prediction performance

Out-of-bag samples

- The bootstrapped training dataset contains n samples drawn at random
- $n - n'$ samples are left out. They are the out-of-bag samples.

- The out-of-bag error can be used to estimate the test error and prediction performance.
- No cross-validation is needed.

Random forest

- Bagging always considers all p variables to build a decision tree.
- Consequently, individual trees in bagging may look very similar.
- Random forest selects at random a subset of m variables to be considered at each split.
- Consequently, individual trees in random forests may look very different (or random).

How to select m?

- Regression random forest: $m = p/3$
- Classification random forest: $m = \sqrt{p}$
- Bagging: $m = p$

Figure 1: Bagging

Figure 2: Random forest

Boosting of trees

- Trees are grown sequentially, using information from previously grown trees.
- Boosting learns from mistakes, after fitting the first tree, further trees are grown based on the residuals.
- Tuning parameters:

    1. B: Number of trees
    2. λ: Learning rate
    3. d: Number of splits per tree, interaction depth

Boosting algorithm

1. Initialise the output parameters: the predicted values $f(x) = 0$ and the residuals $r_i = y_i$ for all observations i.
2. Loop through $b \in 1, ..., B$, repeat:

    1. Fit tree b with d splits, obtain new predicted values $f_b(x)$
    2. Update
    $$f(x) = f(x) + \lambda f_b(x)$$
    3.
    $$r_i = r_i - \lambda f_b(x)$$

3. Output as the final model the boosted predictions

$$f_{boost}(x) = \sum_{b=1}^{B} \lambda f_b(x)$$

Outlook: gradient and XGboost

- Gradient Boosting: A special case of boosting where errors are minimized by gradient descent algorithm.
- eXtreme Gradient Boosting (XGBoost):
  - Boosting algorithm, sequential learning
  - Approximation and regularization
  - Computationally efficient, based on parallel and distributed computing

Variable importance: Understanding how algorithms work

Interpretable machine learning

- Variable importance in ensemble trees allows to rank variables by their importance in the model.

Variable importance: Understanding how algorithms work

There are two approaches for variable importance:

1. **Permutation**: Mean decrease in accuracy
   - First fit the model on the original data and evaluate the prediction error on the out-of-bag samples.
   - Permute variable j, refit the model and re-evaluate the prediction error on the out-of-bag samples.
   - The mean decrease of accuracy after permuting variable j can be used to measure the importance of the jth variable.
2. **Gini-index**: Mean decrease in impurity
   - Record the decrease of impurity every time a tree is split at variable j.
   - Average over all trees.

Bagging and random forests in `randomForest`

```
randomForest(
  x, y, # train data
  xtest = NULL, ytest = NULL, # test data
  ntree = 500, # number of trees to grow
  # number of variables to consider in each tree
  mtry = if (!is.null(y) && !is.factor(y)) max(floor(ncol(x) / 3), 1) else floor(sqrt(ncol
  replace = TRUE, # sample with replacement
  importance = TRUE # computes variable importance
)
```

Bagging and random forests in `randomForest`

`mtry` is number of variables to consider in each tree

- Regression random forest: $m = p/3$
- Classification random forest: $m = \sqrt{p}$
- Bagging: $m = p$

```
data(BostonHousing)

# here, use formula rather than x and y
fit <- randomForest(medv ~ ., data = BostonHousing)
fit
```

```
Call:
 randomForest(formula = medv ~ ., data = BostonHousing)
               Type of random forest: regression
                     Number of trees: 500
No. of variables tried at each split: 4

          Mean of squared residuals: 10.23124
                    % Var explained: 87.88
```

Bagging and random forests in `randomForest`

- `$predicted`: Predicted values
- Classification measures: `$err.rate`, `$confusion`, `$votes`

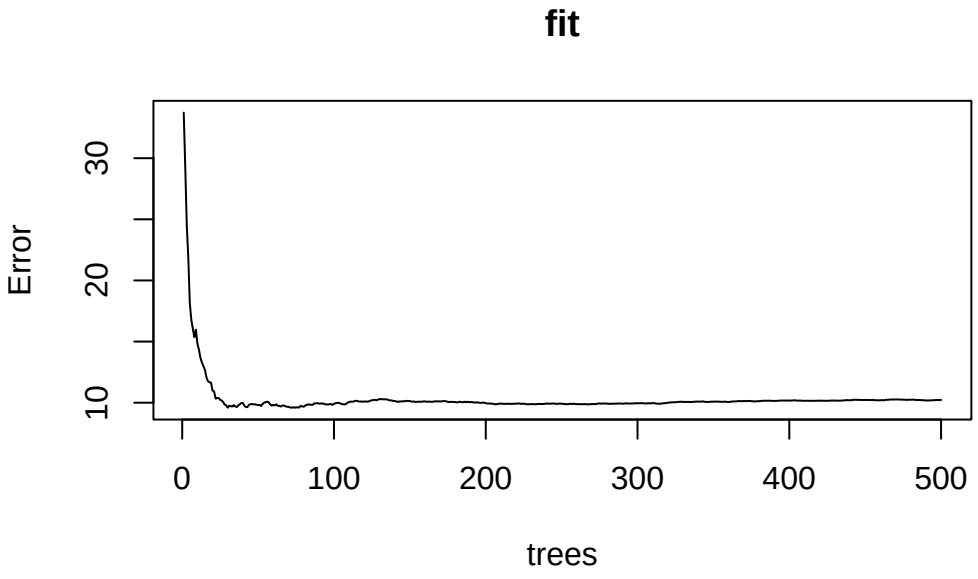
- Regression measures: `$mse, $rsq`
- `$importance`: Variable importance (mean decrease in accuracy and mean decrease in impurity)

Further functions

- `predict.randomForest`: Predict new data
- `plot.randomForest`: Plot error against number of trees
- `varImpPlot`: Plot variable importance

Bagging and random forests in `randomForest`

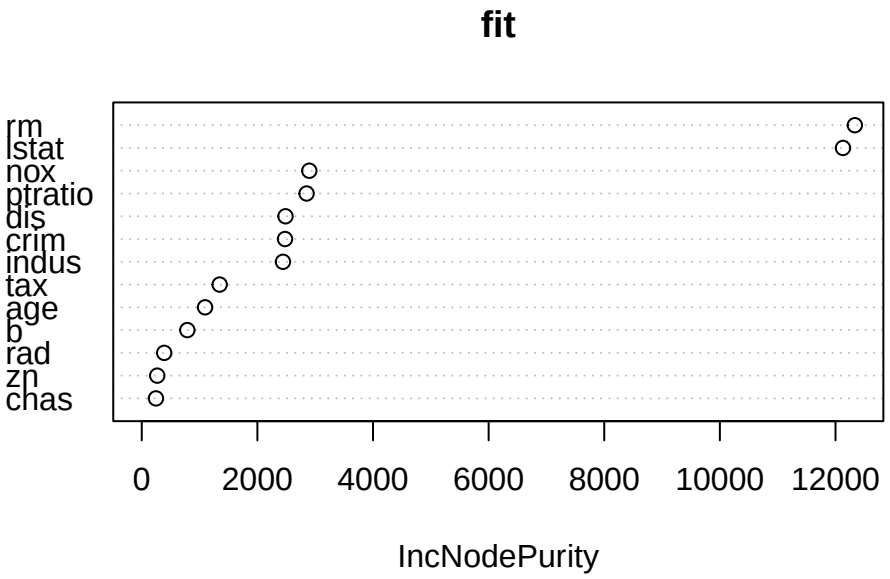
```
plot(fit)
```



Bagging and random forests in `randomForest`

Mean decrease in impurity

```
varImpPlot(fit)
```



Boosting in `gbm`

```
gbm(
  formula,
  distribution, # family of the outcome
  data,
  n.trees = 100, # number of trees to fit
  interaction.depth = 1, # maximum depth of each tree
  n.minobsinnode = 10, # minimum number of observations in the terminal nodes
  shrinkage = 0.1, # shrinkage factor
  cv.folds = 0 # performs additional cross-validation
)
```

Further functions

- `predict.gbm`: Predict new data
- `summary`: Relative influence

Take away: Ensemble methods

- Decision trees offer great interpretability.

- But they tend to overfit, performing poorly in prediction.
- Ensemble methods like bagging, random forest and boosting, fit many trees in different variations and average over them.
- This reduces the variance and leads to greater generalizability.
- Variable importance measures help to understand the contribution of specific variables